CLAIMS

What is claimed is:

1. A method for comparing a query peptide to a plurality of database peptides comprising the steps of:

    (a)   constructing an index table, said index table comprising a plurality of records corresponding to a plurality of allowed mass values, said records comprising zero or more fields, said constructing step comprising the steps of:

        (i)   selecting a first peptide from said plurality of database peptides;

        (ii)   calculating a plurality of associated masses for said first peptide;

        (iii)   selecting a first associated mass from said plurality of associated masses;

        (iv)   referencing a first record from said plurality of records, said first record corresponding to said first associated mass;

        (v)   entering a first field into said first record, said first field comprising a first peptide index referencing said first peptide;

        (vi)   repeating steps (iii)-(v) for at least one other associated mass from said plurality of associated masses;

        (vii)   repeating steps (i)-(vi) for at least one other peptide from said plurality of database peptides; and

    (b)   generating a plurality of comparison scores, said plurality of comparison scores corresponding to said plurality of database peptides, said generating step comprising the steps of:

        (i)   generating a plurality of query mass values for said query peptide;

        (ii)   selecting a first query mass value from said plurality of query mass values;

        (iii)   referencing a second record from said plurality of records, said second record corresponding to said first query mass value;

27   (iv)   selecting a second field from said second record, said second field

28   comprising a second peptide index;

29   (v)   selecting a first comparison score from said plurality of comparison

30   scores, said first comparison score corresponding to said second

31   peptide index;

32   (vi)   incrementing said first comparison score;

33   (vii)   repeating steps (ii)-(vi) for at least one other query mass value

34   selected from said plurality of query mass values.

1   2.   The method of claim 1 wherein said generating step (b)(i) comprises the step of

2   performing mass spectroscopy on said query peptide.

1   3.   The method of claim 2 wherein said mass spectroscopy is performed by a method

2   selected from the set consisting of: Fourier transform ion cyclotron resonance

3   ("FTICR"), quadrupole mass spectroscopy, ion trap mass spectroscopy, and time-

4   of-flight mass spectroscopy.

1   4.   The method of claim 1 wherein said calculating step (a)(ii) comprises the step of

2   calculating a plurality of associated masses for said first peptide, said plurality of

3   associate masses comprising a plurality of primary masses and a plurality of

4   complementary masses.

1   5.   The method of claim 1 wherein said generating step (b) further comprises the step

2   of multiplying said first comparison score by a weight value, wherein said weight

3   value is a function of the type of mass value.

1   6.   The method of claim 5 wherein said type of mass value is selected from the group

2   consisting of: y-ion, b-ion, peak mass, and complementary mass.

1   7.   A method for comparing a query peptide to a plurality of database peptides

2   comprising the steps of:

3 (a) constructing a first index table, said first index table comprising a first

4   plurality of records corresponding to a plurality of allowed mass values,

5   said records comprising zero or more fields; and

6 (b) constructing a second index table, said second index table comprising a

7   second plurality of records corresponding to said plurality of allowed mass

8   values, said records comprising zero or more fields; and

9 (c) calculating a plurality weight values, said weight values set according to

10   the predictive value of said first and second index tables.

1 8. A method for comparing a modified query peptide to a plurality of database

2 peptides comprising the steps of:

3 (a) generating a plurality of query mass values for said query peptide;

4 (b) identifying a set of query mass values from said plurality of query mass

5   values, wherein said set corresponds to modified mass values;

6 (c) determining a spectral range for said query peptide;

7 (d) subdividing said spectral range into a plurality of equal intervals;

8 (e) performing a plurality of searches on said plurality of equal intervals.

1 9. The method of claim 8 further comprising the step of excluding said set of query

2 mass values.

1 10. The method of claim 8 further comprising the step of adjusting said set of query

2 mass values.

1 11. A method for comparing a query peptide to a plurality of database peptides

2 comprising the step of constructing an index table, said index table comprising a

3 plurality of records corresponding to a plurality of allowed mass values, said

4 records comprising zero or more fields, said constructing step comprising the

5 steps of:

6 (i) selecting a first peptide from said plurality of database peptides;

7 (ii) identifying a modification site on said first peptide;

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8	(iii)	applying a modification to said modification site, producing a first modified peptide;
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10	(iv)	calculating a plurality of associated masses for said first modified peptide;
11	(v)	selecting a first associated mass from said plurality of associated masses;
12	(vi)	referencing a first record from said plurality of records, said first record corresponding to said first associated mass;
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14	(vii)	entering a first field into said first record, said first field comprising a first peptide index referencing said first peptide;
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16	(viii)	repeating steps (v)-(vii) for at least one other associated mass from said plurality of associated masses;
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18	(ix)	repeating steps (i)-(viii) for at least one other peptide from said plurality of database peptides.
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1   12.   The method of claim 11 wherein said identification step (ii) comprises the step of

2   identifying a modification site selected from the group consisting of: a

3   phosphorylation site, an oxidation site, and a substitution site.

1   13.   The method of claim 12 wherein said phosphorylation site comprises an amino

2   acid selected from the group consisting of: serine, threonine, and tyrosine.

1   14.   The method of claim 12 wherein said oxidation site comprises an amino acid

2   selected from the group consisting of: cysteine and methionine.

1   15.   The method of claim 12 wherein said substitution site comprises an amino acid

2   selected from the group consisting of: glutamine, glutamate, asparagine, and

3   aspartate.